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13. ABSTRACT *(Maximum 200 words)*

The goals of this research are to give predictive, quantitative models that can be used to improve shape-memory and magnetostrictive materials, and that can guide the development of new materials. A new theory of martensite and a new theory of magnetostriction were found, both of which predict accurately observed domain structures in these alloys. The principal findings based on these theories are 1) the importance of the precise values of the lattice parameters in determining the microstructure, and therefore the behavior of these materials; 2) the presence of the growth twins in $Tb_xDy_{1-x}Fe_2$, the material with the largest known magnetostriction, do not decrease the magnetostrictive strain in this alloy, as was formerly thought; 3) thermoelastic theory gives a mechanism for increased strain-rate dependence in uniaxial tension experiments on TiNi. A unique experimental facility was built for fundamental experimental studies on stress and magnetic field-induced phase transformation.

14. SUBJECT TERMS
Shape-memory materials, magnetostriction, martensite, phase transformations, stress-induced transformation

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Basic Research on the Improvement of Shape-Memory and Magnetostrictive Materials

Richard D. James

October 13, 1993

U. S. Army Research Office

DAAL03-89-G-0081

University of Minnesota

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A. STATEMENT OF THE PROBLEM STUDIED

The goals of this research are to give predictive, quantitative models that can be used to improve current smart materials and that can guide the development of new materials. This research concerns primarily shape-memory materials and magnetostrictive materials, especially those with large magnetostriction.

B. SUMMARY OF THE MOST IMPORTANT RESULTS

We have developed a new theory for the domain structure of $Tb_xDy_{1-x}Fe_2$, the material with the largest room temperature magnetostrictive strain. This theory gives quantitative predictions of the relation between the domain structure and magnetostrictive strain. There are excellent agreements between our predictions and the observations of Lord, including his most recent observations (done after the theory).

During the period of this grant, we have made major improvements in the laboratory. To test the predictions of theory for the domain structure $Tb_xDy_{1-x}Fe_2$, we have installed a magnet, and we have built an optical system for domain observations. We are currently learning how to do surface preparation of magnetoelastic alloys. When completed (during the next few months), we will have a unique facility for direct domain observations under applied stress and magnetic fields. The biaxial loading machine has reached maturity and is yielding a wealth of information on origins of metastability, hysteresis, kinetics and microstructure. We are beginning to study the behavior of thin films (an ideal application for this machine).

Our studies strongly support the idea that that it should be possible to make a magneto-memory material (a magnetostrictive material that undergoes a first-order martensitic transformation). We now have a better idea what symmetry changes, transformation strains and transformation temperatures are desirable. We strongly believe that such a material would have a major impact on applications.

The recent work of Luskin and his group has focussed on the dynamic development of microstructure. Previous studies of the dynamical development of microstructure have focused almost exclusively on one-dimensional models which cannot begin to describe the complexity of real martensitic crystals. We have recently developed numerical methods for the solution of a model for the dynamics of martensitic crystals, and we have used these numerical methods to begin the study of three-dimensional dynamical models and the comparison of their solutions with experimental results.

We have obtained computational results for the dynamical development of a twinned martensitic microstructure from a homogeneous state when a deformation is prescribed on the crystalline boundary (hard loading) for which the twinned microstructure is energetically favored. We have also computed the dynamical behavior of our model for a martensitic crystal with the same homogeneous initial data when the crystal is not constrained on the boundary, but which is traction-free on the boundary (soft loading). In this case, the homogeneous state evolved with a damped, periodic behavior.

We have recently obtained the first computational results for the motion of the austenitic-finely twinned martensitic interface. Experimental observations have shown that for slow cooling the indium-thallium alloy transformed from the face-centered cubic structure (austenitic phase) to the face-centered tetragonal structure (martensitic phase) by the motion of a single planar interface which traversed the crystal from one end to the other. Upon heating, the interface moves back in the opposite direction. In such experiments, it was also reported that interfacial movement ceased when heating or cooling was stopped and that the movement was never completely smooth, but occurred as a series of discontinuous jerks with intermediate pauses. The martensitic region was finely twinned in these experiments. We have successfully simulated these experimental results for the motion of the austenitic-finely twinned martensitic interface in response to cooling and heating. We have also developed innovative techniques for the visualization of microstructure in three-dimensional crystals.

Leo' s work has involved issues related to microstructural design and its impact on macroscopic properties. He worked extensively on coupling mechanical effects with transport phenomena. This work includes studies of two-phase microstructures that arise from diffusional phase transformations in metals and ceramics. Leo's research explores the role of elastic stresses on the formation of these microstructure. His recent results enable one to predict how the size and shape of a single precipitate particle depends on applied stress, and he is currently completing work on a numerical method that can track the growth of multiple precipitates in an arbitrary applied stress field.

A related area of Leo's work relates to transport effects in shape memory alloys. Shape memory materials undergo a diffusionless phase transformation in which the parent and product phases have the same chemical composition but different crystal structures. Shape memory materials exhibit a hysteresis in their stress-strain curve, the origins of which are not well understood. Leo's work focuses on understanding how heat flow during the phase transformation alters the stress-strain behavior of these materials, particularly the hysteresis in their stress-strain curve. This work also provides a physical explanation for the observed velocity of the austenite--martensite interface that can be related to kinetic relations such as those proposed by Abeyaratne and Knowles.

Leo has also worked on problems in composite materials. He has completed work in collaboration with Oscar Bruno on calculating estimates on the elastic moduli of composite materials by using a complex variable method. Leo has also worked on applying such homogenization models to novel composite systems, such as biological materials.

C. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS REPORTING PERIOD, INCLUDING JOURNAL REFERENCES:

a. P. Kloucek and M. Luskin, The computation of the dynamics of martensitic microstructures, preprint.

b. J. M. Ball and R. D. James, Proposed experimental tests of a theory of fine microstructure and the two-well problem, *Phil. Trans. Royal Soc. London* A338 (1992), pp. 389-450.

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d. R. D. James and D. Kinderlehrer, Frustration and microstructure: an example in magnetostriction, *Progress in partial differential equations: calculus of variations, applications* (ed. C. Bandle, J. Benelmans, M. Chipot, M. Grüter, J. St. Jean Paulin). Pitman Research Notes in Mathematics 267, Longmans, 1992.

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t. Xiaoping Liu and R. D. James, Stability of fiber networks under biaxial stretching, submitted to J. Appl. Mech.
u. C. Chu and R. D. James, Biaxial loading experiments on CuAlNi single crystals, Proc. ASME symposium on Experiments in Smart Materials and Structures.

D. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED DURING THIS REPORTING PERIOD:

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REPORT OF INVENTIONS

No patented inventions have yet been made as a result of this grant.